

1,4-Dicyclopropylbuta-1,3-diyne

Inchi:	InChI=1S/C10H10/c1(3-9-5-6-9)2-4-10-7-8-10/h9-10H,5-8H2
InchiKey:	QKYOSKNMZOKGDC-UHFFFAOYSA-N
Formula:	C10H10
SMILES:	C(C#CC1CC1)#CC1CC1
Mol. weight [g/mol]:	130.19
CAS:	114546-62-2

Physical Properties

Property code	Value	Unit	Source
gf	560.42	kJ/mol	Joback Method
hf	440.47	kJ/mol	Joback Method
hfus	24.17	kJ/mol	Joback Method
hvap	41.98	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	1.813		Crippen Method
mcvol	112.840	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	459.68	K	Joback Method
tc	708.70	K	Joback Method
tf	450.54	K	Joback Method
vc	0.433	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.52	J/mol×K	459.68	Joback Method
cpg	245.84	J/mol×K	501.18	Joback Method
cpg	260.86	J/mol×K	542.69	Joback Method
cpg	274.68	J/mol×K	584.19	Joback Method
cpg	287.43	J/mol×K	625.69	Joback Method
cpg	299.21	J/mol×K	667.20	Joback Method
cpg	310.13	J/mol×K	708.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C114546622&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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